ELSEVIER Journal of Computational and Applied Mathematics 61 (1995) 245–261

JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

The Chebyshev methods of Panovsky and Richardson as Runge–Kutta–Nyström methods

John P. Coleman*, Andrew S. Booth

Department of Mathematical Sciences, University of Durham, South Road, Durham, DH1 3LE, United Kingdom

Received 21 September 1993; revised 8 April 1994

Abstract

The two-step methods proposed by Panovsky and Richardson (this journal, 1988) and analysed by Coleman and Booth (this journal, 1992) are shown to be equivalent to certain Runge–Kutta–Nyström methods for differential equations of the form $y'' = f(x, y)$. An important advantage of the new formulation is that it is no longer necessary to provide additional starting values at the beginning of a calculation or when the steplength or the order is changed; the new formulation is also more stable with respect to the propagation of rounding errors.

Keywords: Hybrid methods; Runge–Kutta–Nyström methods; Collocation; Second-order differential equations; Chebyshev methods

1. Introduction

Implicit methods proposed by Panovsky and Richardson [13] for initial-value problems of the form

$$y'' = f(x, y), \qquad y(x_0) = y_0, \qquad y'(x_0) = z_0 \tag{1.1}$$

were analysed by Coleman and Booth [3] who expressed them as two-step hybrid methods. Here it is shown that they are equivalent to certain collocation methods and therefore to Runge–Kutta–Nyström methods. The one-step formulation has important advantages in starting the calculation and in any subsequent changes of steplength or of order.

A generalisation of the Panovsky–Richardson methods is introduced in Section 2. The main purpose of this is to reveal the nature of the equivalence with collocation methods more clearly than an exposition based on the specific formulae of the Panovsky–Richardson methods would allow. Section 3 is concerned with one-step collocation methods for the initial-value problem (1.1); these are known to be a subset of the Runge–Kutta–Nyström methods. In Section 4 we prove that

* Corresponding author.

0377-0427/95/$09.50 © 1995 Elsevier Science B.V. All rights reserved
SSDI 0377-0427(94)00074-3

the methods of the earlier sections are equivalent, in the sense that, in the absence of rounding errors, they would produce identical numerical results from the same starting values. In the presence of rounding errors the Runge–Kutta–Nyström form is found to be preferable to the original form of the Panovsky–Richardson methods; comparisons for some test problems are given in Section 5.

Some negative results are established in Section 6 where we show that Panovsky–Richardson methods are neither P-stable nor symplectic. The long-term behaviour of the global error in these methods is discussed in Section 7.

2. A generalisation of the methods of Panovsky and Richardson

We begin, as in [3], with the identity

$$y(x+th) - 2y(x) + y(x-th) = \int_x^{x+th} (x+th-z)[f(z) + f(2x-z)]\,dz, \tag{2.1}$$

where, for notational convenience, the second argument of the function f is temporarily suppressed. For a fixed steplength h, let $x_k = x_0 + kh$ for $k = 0, 1, \ldots$. Taking $x = x_k$ and letting $z = x_k + sh$ we can write (2.1) as

$$y(x_k+th) - 2y(x_k) + y(x_k-th) = h^2 \int_0^t (t-s)[f^+(s) + f^-(s)]\,ds \tag{2.2}$$

with

$$f^{\pm}(s) = f(x_k \pm sh).$$

Let $f^{\pm}(s)$ be approximated by interpolating polynomials of degree n based on a set of $n+1$ distinct nodes $\{c_j: j = 0, \ldots, n\}$, i.e.,

$$f^{\pm}(s) \simeq \sum_{j=0}^{n} l_j(s) f^{\pm}(c_j),$$

where

$$l_j(s) = \prod_{\substack{i=0 \\ i \neq j}}^{n} \frac{s - c_i}{c_j - c_i} = \frac{\omega_{n+1}(s)}{(s-c_j)\omega'_{n+1}(c_j)} \tag{2.3}$$

with

$$\omega_{n+1}(s) = \prod_{i=0}^{n} (s - c_i).$$

Then, with y_k and $y_{k \pm c_j}$ as approximations for $y(x_k)$ and $y(x_k \pm c_j h)$, respectively, and with

$$f_{k \pm c_j} = f(x_{k \pm c_j}, y_{k \pm c_j}),$$

Eq. (2.2) gives the formulae

$$y_{k+c_i} = 2y_k - y_{k-c_i} + h^2 \sum_{j=0}^{n} B_{ij}(f_{k+c_j} + f_{k-c_j}), \tag{2.4}$$

where

$$B_{ij} = \int_0^{c_i} (c_i - s)\, l_j(s)\, \mathrm{d}s, \quad i, j = 0, \ldots, n. \tag{2.5}$$

If the nodes are arranged in increasing order on $[0, 1]$, with

$$c_0 = 0 < c_1 < \cdots < c_{n-1} < c_n = 1, \tag{2.6}$$

then (2.4) gives a set of n equations from which y_{k+1} and the off-step values y_{k+c_i} $(i = 1, \ldots, n-1)$ may be calculated.

To implement any of these two-step hybrid methods, which we shall call GPR methods, it is necessary to provide starting values at x_0 and x_1, and also at any off-step points between x_0 and x_1. A similar problem arises if the steplength is changed during the calculation.

The Panovsky–Richardson method of degree n, in the notation of [3], is based on the nodes

$$c_i = \tfrac{1}{2}(1 + \alpha_i), \qquad \alpha_i = \cos(n - i)\pi/n, \quad i = 0, 1, \ldots, n. \tag{2.7}$$

With that choice it can be shown that for $j = 1, \ldots, n-1$

$$l_j(t) = \frac{(-1)^{n-j+1}(1 - \alpha^2)\, T_n'(\alpha)}{n^2(\alpha - \alpha_j)}, \tag{2.8}$$

where $\alpha = 2t - 1$ and T_n is the Chebyshev polynomial of degree n. Expressions for $l_0(t)$ and $l_n(t)$ are obtained by halving the right-hand side of (2.8) and substituting the appropriate values for j. Then (2.4) gives Eq. (3.1) of [3] with the coefficients as in (3.6c) of that paper.

The interpolation nodes used in a Panovsky–Richardson method are the images of the extrema α_i of a Chebyshev polynomial, under a linear transformation which maps $[-1, 1]$ onto $[0, 1]$. They have the symmetry property

$$c_{n-i} = 1 - c_i \quad \text{for } i = 0, 1, \ldots, [\tfrac{1}{2}(n-1)]. \tag{2.9}$$

Several other choices, based on the zeros or extrema of orthogonal polynomials, share this symmetry which, through the following lemma, plays an important role in the equivalence to be established in Section 4.

Lemma 1. *If the set of real numbers* $\{c_j\}$ *satisfies conditions* (2.6) *and* (2.9) *then*

$$B_{nj} + B_{nn-j} = \int_0^1 l_j(s)\, \mathrm{d}s \tag{2.10}$$

for $j = 0, 1, \ldots, n$.

Proof. From (2.3) we can write

$$l_{n-j}(s) = \prod_{\substack{i=0 \\ i \neq j}}^{n} \frac{s - c_{n-i}}{c_{n-j} - c_{n-i}} = \prod_{\substack{i=0 \\ i \neq j}}^{n} \frac{(1-s) - c_i}{c_j - c_i} = l_j(1-s). \tag{2.11}$$

Consequently,

$$B_{nn-j} = \int_0^1 (1-s)\, l_j(1-s)\, \mathrm{d}s = \int_0^1 t\, l_j(t)\, \mathrm{d}t,$$

by an obvious change of integration variable, and (2.10) follows. □

3. One-step collocation methods

A one-step collocation method for the initial-value problem (1.1) involves approximating the solution on the interval $[x_k, x_{k+1}]$ by a polynomial which satisfies the differential equation at a set of $n+1$ collocation points $\{x_{k+c_j} = x_k + c_j h : j = 0, \ldots, n\}$. The number and the labelling of points are chosen for consistency with Section 2. It will be assumed that $c_0 < c_1 < \cdots < c_n$.

Let u be the polynomial of degree $n+2$ such that

$$u''(x_{k+c_j}) = f(x_{k+c_j}, u(x_{k+c_j})), \quad j = 0, \ldots, n, \tag{3.1}$$

with $u(x_k) = y_k$ and $u'(x_k) = z_k$, where y_k and z_k are, respectively, approximations for $y(x_k)$ and $y'(x_k)$. Then the required approximations for $y(x_{k+1})$ and $y'(x_{k+1})$ are $y_{k+1} = u(x_{k+1})$ and $z_{k+1} = u'(x_{k+1})$. Properties of such collocation methods have been discussed in [2, 4, 9, 10, 15].

For arbitrary distinct collocation points

$$u''(x_k + th) = \sum_{j=0}^{n} l_j(t)\, u''(x_{k+c_j}), \tag{3.2}$$

where l_j is a cardinal polynomial for Lagrange interpolation on the set of points $\{c_i\}$, as in (2.3). Integration gives

$$u'(x_k + th) = z_k + h \sum_{j=0}^{n} \alpha_j(t)\, u''(x_{k+c_j}) \tag{3.3}$$

and

$$u(x_k + th) = y_k + thz_k + h^2 \sum_{j=0}^{n} \beta_j(t)\, u''(x_{k+c_j}), \tag{3.4}$$

where

$$\alpha_j(t) = \int_0^t l_j(s)\, \mathrm{d}s$$

and

$$\beta_j(t) = \int_0^t \int_0^s l_j(\sigma)\, \mathrm{d}\sigma\, \mathrm{d}s = \int_0^t (t-s)\, l_j(s)\, \mathrm{d}s.$$

Writing $u(x_{k+c_i})$ as y_{k+c_i} and, in accordance with (3.1), denoting $u''(x_{k+c_j})$ by f_{k+c_j}, we obtain from (3.4)

$$y_{k+1} = y_k + hz_k + h^2 \sum_{j=0}^{n} b_j f_{k+c_j} \tag{3.5}$$

and for $i = 0, \ldots, n$,

$$y_{k+c_i} = y_k + hc_i z_k + h^2 \sum_{j=0}^{n} B_{ij} f_{k+c_j} \tag{3.6}$$

with

$$b_j = \beta_j(1) = \int_0^1 (1-s)\, l_j(s)\, \mathrm{d}s \tag{3.7}$$

and

$$B_{ij} = \beta_j(c_i) = \int_0^{c_i} (c_i - s)\, l_j(s)\, \mathrm{d}s \tag{3.8}$$

as in (2.5). Similarly, from Eq. (3.3),

$$z_{k+1} = z_k + h \sum_{j=0}^{n} d_j f_{k+c_j} \tag{3.9}$$

with

$$d_j = \alpha_j(1) = \int_0^1 l_j(s)\, \mathrm{d}s. \tag{3.10}$$

Eqs. (3.5), (3.6) and (3.9) describe an $(n+1)$-stage Runge–Kutta–Nyström method with the Butcher tableau (see, for example, [15])

$\boldsymbol{c}$	$\boldsymbol{B}$
	$\boldsymbol{b}^{\mathrm{T}}$
	$\boldsymbol{d}^{\mathrm{T}}$

where $\boldsymbol{B}$ is the $(n+1)\times(n+1)$ matrix with elements B_{ij}, the elements of the vectors $\boldsymbol{b}$ and $\boldsymbol{d}$ are given by (3.7) and (3.10) and $\boldsymbol{c} = (c_0, c_1, \ldots, c_n)^{\mathrm{T}}$. We shall refer to these collocation-based Runge–Kutta–Nyström methods as CRKN methods.

The nodes of a symmetric collocation method satisfy conditions (2.9), in which case we have the following result which is used in Section 4.

Lemma 2. *The approximations determined by a symmetric collocation method satisfy the equations*

$$c_i h z_{k+1} = y_{k+1} - y_{k+c_{n-i}} + h^2 \sum_{j=0}^{n} B_{ij} f_{k+c_{n-j}}$$

for $i = 1, \ldots, n$ *and* $k = 0, 1, \ldots$.

Proof. By integrating Eq. (3.2) twice on $(t,1)$, using the initial conditions $u'(x_{k+1}) = z_{k+1}$ and $u(x_{k+1}) = y_{k+1}$, we obtain

$$(1-t)hz_{k+1} - y_{k+1} + u(x_k + th) = h^2 \sum_{j=0}^{n} \int_t^1 (s-t)\, l_j(s)\,\mathrm{d}s f_{k+c_j}.$$

In particular, if $t = c_{n-i}$ then $1 - t = c_i$ and

$$\int_{1-c_i}^{1} (s - 1 + c_i)\, l_j(s)\,\mathrm{d}s = \int_0^{c_i} (c_i - p)\, l_j(1-p)\mathrm{d}p = B_{in-j}$$

from (2.10) and (2.5). The required result follows. □

4. The equivalence of GPR and CRKN methods

The only starting values required by the CRKN methods of Section 3 are the values y_0 and z_0 contained in the statement of the initial-value problem (1.1). For the GPR methods of Section 2, however, it is necessary to provide a procedure for computing the $n-1$ additional values $\{y_{c_i}: i = 1, \ldots, n-1\}$. One way to do this is by carrying out a single step of a collocation method with the appropriate nodes. We prove here that in that case the GPR method and the corresponding CRKN method are identical.

Theorem 3. *Let* $\{c_j: j = 0, \ldots, n\}$ *be a set of distinct numbers in* $[0,1]$ *such that* $c_0 = 0 < c_1 < \cdots < c_n = 1$ *and* $c_{n-j} = 1 - c_j$ *for* $j = 0, 1, \ldots, [\frac{1}{2}(n-1)]$. *Two numerical methods of fixed steplength* h *are based on the parameter set* $\{c_j\}$, *the GPR method defined by* (2.4) *and the CRKN given by* (3.6) *and* (3.9). *If the starting values provided for the former method are the approximations generated by the latter method on* $[x_0, x_1]$, *the two methods would give identical results at all subsequent steps if the arithmetic could be done exactly.*

Proof. Eq. (2.4) with $i = n$ may be written as

$$y_{k+1} = y_k + hw_k + h^2 \sum_{j=0}^{n} B_{nj} f_{k+c_j}, \tag{4.1}$$

by simply introducing

$$hw_k = y_k - y_{k-1} + h^2 \sum_{j=0}^{n} B_{nj} f_{k-c_j}.$$

Replacing k by $k+1$ in this definition and using (4.1) again we obtain

$$hw_{k+1} = hw_k + h^2 \sum_{j=0}^{n} B_{nj} (f_{k+1-c_j} + f_{k+c_j})$$

and therefore

$$w_{k+1} = w_k + h \sum_{j=0}^{n} (B_{nj} + B_{nn-j}) f_{k+c_j} = w_k + h \sum_{j=0}^{n} d_j f_{k+c_j} \tag{4.2}$$

by Lemma 1 and Eq. (3.10). The Eqs. (4.1) and (4.2) have the same form as Eqs. (3.5) and (3.9) of the corresponding collocation method, but the off-step values arising in the two sets of equations could be different.

More generally, we may write (2.4) as

$$y_{k+c_i} = y_k + hc_i w_k^{(i)} + h^2 \sum_{j=0}^{n} B_{ij} f_{k+c_j}, \tag{4.3}$$

$$hc_i w_k^{(i)} = y_k - y_{k-c_i} + h^2 \sum_{j=0}^{n} B_{ij} f_{k-c_j} \tag{4.4}$$

and, in particular, $w_k^{(n)} = w_k$ as defined previously. Eq. (4.3) differs from (3.6) only in the appearance of $w_k^{(i)}$ instead of z_k. Whereas the CRKN method uses the approximation z_k for $y'(x_k)$ at all stages in the step from x_k to x_{k+1}, the GPR method uses $w_k^{(i)}$ as an approximation for $y'(x_k)$ in the equation for the ith stage. We shall now show that, under the conditions of the theorem, $w_k^{(i)}$ is independent of i; the same derivative approximation is used at every stage, as in the collocation method.

It is evident from (4.4) that $w_k^{(i)}$, used in the step from x_k to x_{k+1}, is determined, for each value of the index i, by quantities which are known at the end of the preceding step. Consider the first step of a GPR method, from x_1 to x_2, with starting values $\{y_{c_i}\}$ given by the CRKN formula (3.6) with $k = 0$. Then Lemma 2 and the defining equation (4.4) show that

$$w_1^{(i)} = z_1 \quad \text{for } i = 1, \ldots, n.$$

The set of equations (4.3) is identical to the set (3.6) and the two methods give identical approximations y_{1+c_i} for $i = 1, \ldots, n$. Entering the next step, the collocation method uses z_2 calculated from (3.9) whereas the GPR method uses $\{w_2^{(i)}\}$. However, Lemma 2 now shows that $w_2^{(i)} = z_2$ and the two methods give identical results on $[x_2, x_3]$. The proof is completed by induction on the step-number k. □

The equivalence established here also holds for variable-steplength computations if the CRKN method is used to provide the necessary starting values for the GPR method each time the steplength is altered. Of the two equivalent formulations the CRKN version is preferable on the grounds of ease of starting the calculation and of varying the steplength or the order of the method.

5. The propagation of rounding errors

In carrying out the calculations reported in [3] we found that the effects of rounding errors can build up rapidly in the Panovsky–Richardson methods. This is also evident from Figs. 1 and 2 of [13], in the changes seen in the error curves around 10^{-12}. It turns out that, in addition to its other benefits, the CRKN formulation is much better in this respect.

There are many instances of mathematically equivalent formulations of a numerical method producing very different numerical results. Hairer et al. [6, p. 430] applied the Störmer formula

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(13f_n - 2f_{n-1} + f_{n-2}),$$

as it is written and in an equivalent one-step formulation, to $y'' = -y$. The effects of rounding error are much more severe in the original version. This is attributed to the fact that whereas the recurrence relation (5.1) is unstable as $h \to 0$, because of the root of multiplicity 2 on the unit circle, the iteration matrix of the one-step formulation is power bounded. Also Henrici [7, Section 6.4] pointed out the superiority of the so-called "summed form" of the Störmer–Cowell methods. Because of the structural similarity of the Störmer–Cowell methods and the GPR methods of Section 2, it is to be expected that here also the one-step formulation would be the more stable with respect to the propagation of rounding error. The re-formulated methods of Henrici [7] and of Hairer et al. [6] may be interpreted as one-step methods but they require the same number of starting values as the original methods; the benefit lies in their response to rounding errors and they lack the other advantages of the equivalence established in Theorem 3.

The Panovsky–Richardson methods may be formulated as in Eq. (20) of [13], in the two-step hybrid form of Eq. (3.1) of [3], or as in Eqs. (3.6) and (3.9) above with $\{c_j\}$ given by (2.7). In exact arithmetic the three forms would yield identical results. Since we have seen no significant differences in the numerical results given by the first two versions we concentrate on comparisons of the two-step form of [3] and the equivalent, one-step, Runge–Kutta–Nyström method. For all the calculations reported here, steplengths were chosen so that the global truncation error on the interval considered is less than the unit round-off in the arithmetic used. We have also confirmed that our conclusions are not affected by reasonable changes in the tolerance parameter for the iterations necessary to solve the implicit equations at each step.

5.1. *Harmonic oscillator*

The sixth-order Panovsky–Richardson method of degree 4 (which we shall denote by PR4) and the equivalent Runge–Kutta–Nyström method (RKN6) were used to solve the initial-value problem

$$y'' = -y, \qquad y(0) = 1, \qquad y'(0) = 0. \tag{5.1}$$

For the fixed steplength $h = 0.01$, computations in quadruple precision show that the magnitude of the global truncation error is less than $5{\cdot}10^{-18}$ on $[0, 10]$ and less than $6{\cdot}10^{-17}$ on $[0, 100]$. The results shown in Fig. 1 were produced by MATLAB programs on a microcomputer. The same programs gave almost identical results on a SUN workstation.

Table 1 compares the results of PR4 and RKN6 on the interval $[0, 100]$, in a variety of computing environments. The MATLAB programs used a Gauss–Seidel-type iterative scheme for the equations which have to be solved at each step (see [3, Section 6]), whereas the Fortran programs used Newton iteration. The entries in Table 1, which are due solely to the propagation of rounding errors, show how much more stable the one-step formulation is for this problem; they also show the inferior quality of the arithmetic on the mainframe computer.

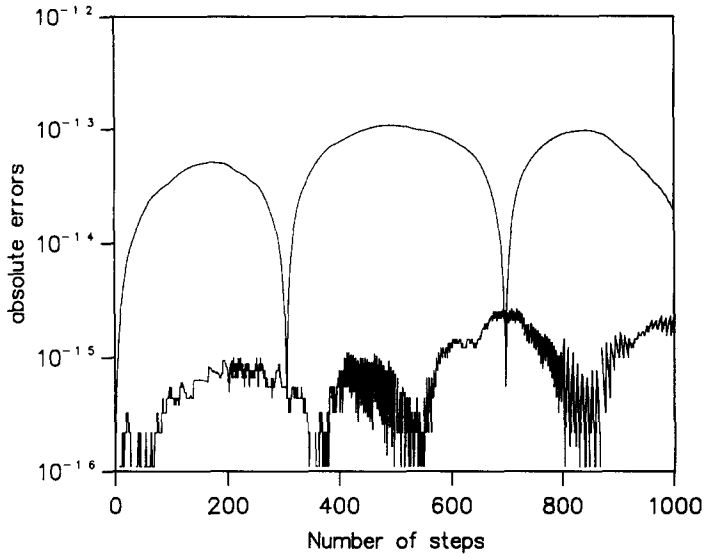

Fig. 1. Absolute errors for PR4 and RKN6 (jagged curve) applied to problem (5.1) with steplength $h = 0.01$.

Table 1
The maximum absolute errors on intervals $[0, x]$ when the equivalent methods PR4 and RKN6 are applied to the initial-value problem (5.1) with steplength $h = 0.01$

x	MATLAB SUN workstation		Fortran double precision			
			SUN workstation		Amdahl mainframe	
	PR4	RKN6	PR4	RKN6	PR4	RKN6
1.0	$3.4\cdot10^{-14}$	$5.6\cdot10^{-16}$	$1.7\cdot10^{-14}$	$4.4\cdot10^{-16}$	$4.9\cdot10^{-13}$	$1.2\cdot10^{-15}$
2.0	$5.2\cdot10^{-14}$	$9.4\cdot10^{-16}$	$6.8\cdot10^{-14}$	$4.4\cdot10^{-16}$	$1.1\cdot10^{-12}$	$1.6\cdot10^{-15}$
5.0	$1.1\cdot10^{-13}$	$1.1\cdot10^{-15}$	$9.0\cdot10^{-14}$	$1.1\cdot10^{-15}$	$3.0\cdot10^{-12}$	$5.8\cdot10^{-15}$
10.0	$1.1\cdot10^{-13}$	$2.7\cdot10^{-15}$	$9.1\cdot10^{-14}$	$2.8\cdot10^{-15}$	$5.0\cdot10^{-12}$	$1.7\cdot10^{-14}$
20.0	$2.4\cdot10^{-13}$	$4.4\cdot10^{-15}$	$1.0\cdot10^{-13}$	$2.9\cdot10^{-15}$	$1.2\cdot10^{-11}$	$3.3\cdot10^{-14}$
50.0	$4.6\cdot10^{-13}$	$7.9\cdot10^{-15}$	$2.2\cdot10^{-13}$	$1.2\cdot10^{-14}$	$3.1\cdot10^{-11}$	$8.7\cdot10^{-14}$
100.0	$4.6\cdot10^{-13}$	$1.2\cdot10^{-14}$	$5.0\cdot10^{-13}$	$1.3\cdot10^{-14}$	$6.3\cdot10^{-11}$	$1.7\cdot10^{-13}$

Table 2, which is based on MATLAB computations, illustrates the effects of different steplengths used over a given number of steps. Identical results were obtained from Panovsky–Richardson methods of higher order.

5.2. *Two-body problem*

A non-linear example is provided by the two-body problem

$$\begin{aligned} &y'' + y/r^3 = 0, \qquad y(0) = 1 - e, \qquad y'(0) = 0, \\ &z'' + z/r^3 = 0, \qquad z(0) = 0, \qquad z'(0) = \sqrt{(1+e)/(1-e)}, \end{aligned} \tag{5.2}$$

Table 2
The maximum absolute errors in 1000 steps when the equivalent methods PR4 and RKN6 are applied to (5.1) with steplength h

h	PR4	RKN6
0.01	$1.1 \cdot 10^{-13}$	$2.7 \cdot 10^{-15}$
0.005	$2.1 \cdot 10^{-13}$	$2.1 \cdot 10^{-15}$
0.002	$3.3 \cdot 10^{-13}$	$8.3 \cdot 10^{-16}$
0.001	$1.1 \cdot 10^{-12}$	$3.6 \cdot 10^{-15}$

Table 3
As Table 1 but for the two-body problem with $e = 0.1$

h	PR4	RKN6
1.0	$1.2 \cdot 10^{-14}$	$1.0 \cdot 10^{-15}$
2.0	$2.2 \cdot 10^{-14}$	$4.2 \cdot 10^{-15}$
5.0	$2.1 \cdot 10^{-13}$	$2.8 \cdot 10^{-14}$
10.0	$6.9 \cdot 10^{-13}$	$5.1 \cdot 10^{-14}$
20.0	$1.4 \cdot 10^{-12}$	$1.2 \cdot 10^{-13}$
50.0	$1.4 \cdot 10^{-11}$	$2.3 \cdot 10^{-13}$
100.0	$2.5 \cdot 10^{-11}$	$1.1 \cdot 10^{-12}$

with $r^2 = y^2 + z^2$. Table 3 shows how rounding errors accumulate in Fortran double-precision computations for this problem, when the equivalent methods PR4 and RKN6 are used with the fixed steplength $h = 0.01$. These results were produced by a SUN workstation. In this case the maximum magnitude of the truncation error on $[0, 10]$, determined by quadruple-precision calculations, is approximately $3 \cdot 10^{-16}$, and on $[0, 100]$ it is less than $5 \cdot 10^{-15}$.

5.3. *A stiff problem*

The initial-value problem

$$\begin{aligned} y'' &= 2498y + 4998z, \qquad y(0) = 2, \qquad y'(0) = 0, \\ z'' &= -2499y - 4999z, \qquad z(0) = -1, \qquad z'(0) = 0, \end{aligned} \tag{5.3}$$

used by Kramarz [9], has the unique solution

$$y(x) = 2\cos x, \qquad z(x) = -\cos x.$$

The initial conditions eliminate the terms $\cos 50x$ and $\sin 50x$ which occur in the general solution of this pair of differential equations. Table 4 provides a numerical comparison of the mathematically equivalent methods PR4 and RKN6, with the fixed steplength $h = 0.01$. Here, as in other examples,

Table 4
As Table 1 but for problem (5.3)

h	PR4	RKN6
1.0	$6.8 \cdot 10^{-14}$	$1.1 \cdot 10^{-15}$
2.0	$1.0 \cdot 10^{-13}$	$1.9 \cdot 10^{-15}$
5.0	$2.2 \cdot 10^{-13}$	$2.2 \cdot 10^{-15}$
10.0	$2.2 \cdot 10^{-13}$	$5.8 \cdot 10^{-15}$
20.0	$4.6 \cdot 10^{-13}$	$1.4 \cdot 10^{-14}$
40.0	$6.4 \cdot 10^{-13}$	$2.3 \cdot 10^{-14}$
80.0	$9.0 \cdot 10^{-13}$	$4.3 \cdot 10^{-14}$

the rounding errors introduced depend on details of the particular implementation of each algorithm. For this comparison, both MATLAB programs used a Gauss–Seidel-type iterative scheme with the same stopping criterion; this scheme is satisfactory for the chosen value of h, but for substantially larger steplengths it would not converge (see [3, Section 6]). The first step was carried out in exactly the same way in both programs; subsequent steps of PR4 were based on Eq. (2.4), whereas Eqs. (3.5), (3.6) and (3.9) provided the basis for RKN6. Once again the superiority of the one-step formulation with respect to the propagation of rounding error is evident. Quadruple-precision computations show that the global truncation error on $[0, 80]$ is less than 10^{-16}.

6. Panovsky–Richardson methods are neither P-stable nor symplectic

Coleman and Booth [3] investigated the stability properties of the Panovsky–Richardson methods of degree n up to 20. The results show that for practical values of n there are no P-stable methods within that family. In view of the equivalence proved in Section 4 we can now extend that statement to all values of n and generalise it to apply to all GPR methods.

Theorem 4. *Generalised Panovsky–Richardson methods are not P-stable for any choice of interpolation nodes.*

Proof. The stability analysis of Coleman and Booth [3] was devised for the Panovsky–Richardson methods but it does not rely on a specific choice of nodes. With the appropriate interpretation of the matrix B, the analysis applies to all GPR methods. Furthermore, the analysis of [3] makes no reference to a particular choice of starting values, so it applies to CRKN methods as to any other implementation of the GPR formulae. Since Coleman [2] has shown that there are no P-stable symmetric one-step collocation methods (i.e., no P-stable CRKN methods), the result follows. □

Several authors have investigated symplectic (also called canonical) numerical integration methods which are of interest in connection with the integration of Hamiltonian systems; Ref. [14] provides a good survey. It has been shown that a Runge–Kutta–Nyström method without

redundant stages is canonical if and only if, in the notation of Section 3,

$$b_i = (1 - c_i)d_i, \quad 0 \leqslant i \leqslant n \tag{6.1}$$

and

$$d_j(b_i - B_{ji}) = d_i(b_j - B_{ij}), \quad 0 \leqslant i < j \leqslant n. \tag{6.2}$$

A derivation of these conditions, which are attributed to Suris, may be found in [12].

Theorem 5. *The Panovsky–Richardson methods are not symplectic.*

Proof. (a) *The first set of conditions of Suris*: From Eqs. (3.7), (3.10) and (2.3),

$$b_i - (1 - c_i)d_i = -\frac{1}{\omega'_{n+1}(c_i)} \int_0^1 \omega_{n+1}(s)\,\mathrm{d}s.$$

For symmetric nodes,

$$\omega_{n+1}(1 - s) = (-1)^{n+1}\omega_{n+1}(s)$$

and consequently (6.1) is satisfied when n is even. In other words, every symmetric CRKN method with an odd number of stages satisfies the first set of conditions; for an even number of stages (n odd) symmetry considerations do not help and the answer depends on the particular choice of collocation nodes.

In the case of the Panovsky–Richardson methods it is convenient to let $s = \frac{1}{2}(1 + \alpha)$ with $c_i = \frac{1}{2}(1 + \alpha_i)$, where $\alpha_i = \cos(n - i)\pi/n$. Then for odd values of n

$$\int_0^1 \omega_{n+1}(s)\,\mathrm{d}s = \frac{-1}{n2^{2n+1}} \int_{-1}^1 (1 - \alpha^2)\,T'_n(\alpha)\,\mathrm{d}\alpha$$

$$= \frac{1}{n(n^2 - 4)2^{2n-1}}$$

by integration by parts and use of some elementary properties of the Chebyshev polynomials. It follows that the Panovsky–Richardson methods of odd degree are not symplectic.

(b) *The second set of conditions*: Here it will be assumed that conditions (6.1) are satisfied and that n is even. If $c_n = 1$ then, from (3.8) and (3.7),

$$B_{ni} = b_i, \quad i = 0, 1, \ldots, n$$

and (6.1) with $i = n$ gives

$$b_n = 0.$$

Then the set of conditions corresponding to the choice $j = n$ in (6.2) reduces to

$$d_i B_{in} = 0, \quad i = 0, 1, \ldots, n. \tag{6.3}$$

We shall show that both B_{1n} and d_1 are nonzero for the Panovsky–Richardson methods.

Eq. (3.8) gives

$$B_{1n} = \int_0^{c_1} (c_1 - s) l_j(s)\,\mathrm{d}s \neq 0$$

since the integrand is of constant sign on $(0, c_1)$.

The polynomial of degree n which interpolates a function g at the extrema of $T_n(\alpha)$ is

$$p_n(\alpha) = \sum_{j=0}^{n}{}'' A_j T_j(\alpha),$$

where

$$A_j = \frac{2}{n} \sum_{i=0}^{n}{}'' g(\alpha_i) T_j(\alpha_i)$$

and the double prime on the sum indicates that the first and last terms are to be halved (see e.g., [5, p. 32]). If $g(\alpha_1) = 1$ and $g(\alpha_i) = 0$ for $i = 0, 2, 3, \ldots, n$ then

$$p_n(\alpha) = \tilde{l}_1(x) = \frac{\tilde{\omega}_{n+1}(\alpha)}{(\alpha - \alpha_1)\tilde{\omega}'(\alpha_1)}, \tag{6.4}$$

where

$$\tilde{\omega}_{n+1}(\alpha) = \prod_{i=0}^{n} (\alpha - \alpha_i)$$

and α_i is as in part (a) of this proof. In that case

$$A_j = \frac{2}{n} T_j(\alpha)$$

and consequently

$$\tilde{l}_1(\alpha) = \frac{2}{n} \sum_{j=0}^{n}{}'' T_j(\alpha_1) T_j(\alpha).$$

Comparison of (2.3) and (6.4), when combined with the defining equation (3.10), shows that, with $n = 2k$,

$$\begin{aligned} d_1 &= \frac{1}{2} \int_{-1}^{1} \tilde{l}_1(\alpha)\,\mathrm{d}\alpha \\ &= \frac{1}{n} \sum_{j=0}^{n}{}'' T_j(\alpha_1) \int_{-1}^{1} T_j(\alpha)\,\mathrm{d}\alpha \\ &= \frac{1}{n}\left[1 - \sum_{i=1}^{k-1} \frac{2}{4i^2 - 1} T_{2i}(\alpha_1) - \frac{1}{n^2 - 1} T_n(\alpha_1)\right]. \end{aligned}$$

Since

$$T_{2i}(\alpha) = \cos\frac{i\pi}{k}$$

we obtain

$$d_1 = \frac{1}{n}\left[1 - 2\sum_{i=1}^{k-1}\frac{\cos i\pi/k}{4i^2-1} + \frac{1}{n^2-1}\right].$$

Now we note that

$$2\left|\sum_{i=1}^{k-1}\frac{\cos i\pi/k}{4i^2-1}\right| \leqslant \sum_{i=1}^{k-1}\left(\frac{1}{2i-1} - \frac{1}{2i+1}\right) = 1 - \frac{1}{2k+1} < 1$$

with the consequence that $d_1 > 0$.

Since (6.3) does not hold with $i = 1$ none of the Panovsky–Richardson methods is symplectic. □

Apart from a factor of 2, the numbers d_j are the weights of a Clenshaw–Curtis quadrature formula. The conclusion that $d_1 > 0$ is therefore a special case of the fact, proved by Imhof [8], that the Clenshaw–Curtis weights are all positive.

7. The long-term behaviour of the global truncation order

Theorem 5 raises an interesting question. Calvo and Sanz-Serna [1] used two Runge–Kutta–Nyström methods, one symplectic and the other not, to solve the two-body problem (5.2). The global error of the symplectic method was approximately linear in time, whereas that of the other method ultimately increased approximately quadratically. However, in [3] we remarked on the near-linear behaviour of the global error in the Panovsky–Richardson methods applied to the same problem, and contrasted it with the quadratic increase in the global error of a particular explicit Runge–Kutta–Nyström method. Having established that the Panovsky–Richardson methods are Runge–Kutta–Nyström methods and are not symplectic, we undertook a more detailed investigation of the long-term behaviour of the Panovsky–Richardson methods for the two-body problem.

Calvo and Sanz-Serna [1] examined the asymptotic form of the global error of a one-step method of order p applied, with a fixed steplength, to problem (5.2). They concluded that the error after N complete periods has the form

$$\boldsymbol{E}_N = N\boldsymbol{E}_1 + \tfrac{1}{2}(N^2 - N)(\boldsymbol{G}_0^{\mathrm{T}}\boldsymbol{E}_1)\boldsymbol{W}_0 + \mathrm{O}(h^{2p}), \tag{7.1}$$

where $\boldsymbol{E}_1$ is the error vector at the end of the first period, $\boldsymbol{G}_0$ is the initial energy gradient and the precise form of the vector $\boldsymbol{W}_0$ need not concern us here. This leads to the expectation that, in general, $\boldsymbol{E}_N$ will ultimately grow quadratically with N. Of course the coefficient of the quadratic term will usually depend on the steplength h; the nature of the dependence and the magnitude of that term will depend on the particular numerical method used. Calculations of Calvo and Sanz-Serna [1], based on a fourth-order explicit Runge–Kutta–Nyström method, showed an approximately quadratic increase in the global error, as did our calculations [3] with an explicit Runge–Kutta–Nyström method of order 8.

Calvo and Sanz-Serna [1] also showed that for symplectic methods the second term on the right-hand side of Eq. (7.1) only contributes to the $O(h^{2p})$ term, with the result that

$$E_N = NE_1 + O(h^{2p}).$$

In so far as the $O(h^{2p})$ terms may be ignored, the global error after N periods, for a one-step symplectic method applied to Kepler's problem with a constant steplength, grows linearly with N. However, the analysis of Calvo and Sanz-Serna [1] does not seem to preclude a similar behaviour for some nonsymplectic method, despite their statement that "for nonlinear oscillators standard methods have quadratic error growth and symplectic methods produce errors that grow only linearly".

We applied several Panovsky–Richardson methods, in Runge–Kutta–Nyström form, with a variety of different steplengths and eccentricity values, over time intervals of up to 65 610 orbital periods. Mostly small values of the eccentricity were used since fixed-steplength computations of reasonable accuracy over a large number of orbits would otherwise require a prohibitively large amount of computation. Errors were recorded after specified numbers of complete orbits, when the exact solution is given by the initial conditions imposed in (5.2). Table 5 and Fig. 2 show the behaviour of the method RKN6, the RKN method which is equivalent to the Panovsky–Richardson method of degree 4, and therefore of order 6. The error norm, chosen for consistency with [1], is the Euclidean norm of the four-dimensional vector whose components are the errors in the approximations for y, y', z and z'.

In Fig. 2, for the smaller steplengths, the rate of increase in the error norm is very close to linear over the full range of 65 610 orbits, as is also evident from the last column of Table 5 for the

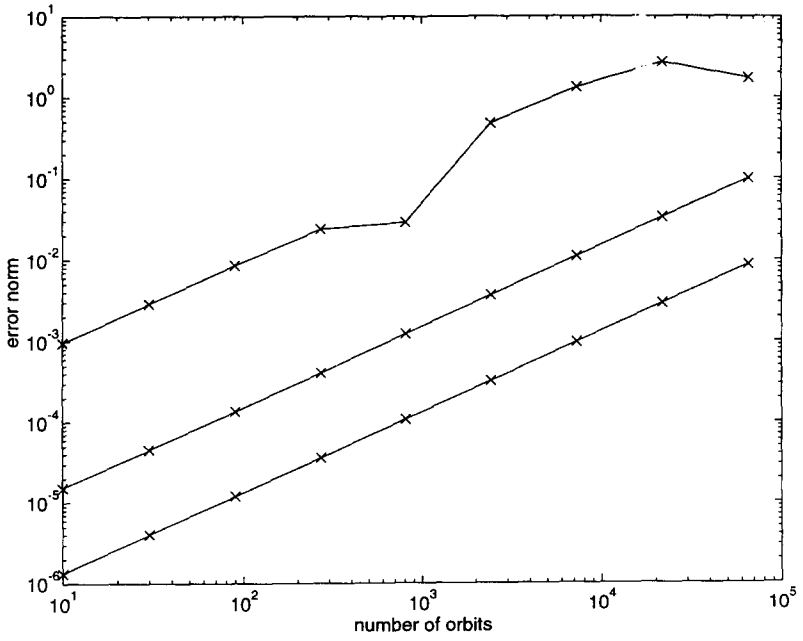

Fig. 2. The error norm after $10 \cdot 3^n$ orbits ($n = 0, 1, \ldots, 8$) when the method RKN6 is applied to problem (5.2) with $e = 0.1$ and steplengths $h = \frac{1}{12}\pi$, $\frac{1}{8}\pi$ and $\frac{1}{4}\pi$.

Table 5
Results for the sixth order method RKN6 applied to problem (5.2) with $e = 0.1$ and steplength $h = \frac{1}{8}\pi$

Number of orbits	Error in y value	Error in z value	Error norm	Ratio of error norms
10	$2.8 \cdot 10^{-11}$	$1.10 \cdot 10^{-5}$	$1.51 \cdot 10^{-5}$	
30	$2.5 \cdot 10^{-10}$	$3.31 \cdot 10^{-5}$	$4.55 \cdot 10^{-5}$	3.000
90	$2.2 \cdot 10^{-9}$	$9.93 \cdot 10^{-5}$	$1.37 \cdot 10^{-4}$	3.000
270	$2.0 \cdot 10^{-8}$	$2.98 \cdot 10^{-4}$	$4.10 \cdot 10^{-4}$	3.000
810	$1.8 \cdot 10^{-7}$	$8.94 \cdot 10^{-4}$	$1.23 \cdot 10^{-3}$	3.000
2430	$1.6 \cdot 10^{-6}$	$2.68 \cdot 10^{-3}$	$3.69 \cdot 10^{-3}$	3.000
7290	$1.5 \cdot 10^{-5}$	$8.05 \cdot 10^{-3}$	$1.11 \cdot 10^{-2}$	3.000
21870	$1.3 \cdot 10^{-4}$	$2.41 \cdot 10^{-2}$	$3.32 \cdot 10^{-2}$	2.999
65610	$1.2 \cdot 10^{-3}$	$7.22 \cdot 10^{-2}$	$9.92 \cdot 10^{-2}$	2.990

steplength $\frac{1}{8}\pi$. After any given number of orbits, the ratio of the error norm obtained with $h = \frac{1}{8}\pi$ to that for $h = \frac{1}{12}\pi$ is 11.4, to three significant figures, in agreement with the value $(1.5)^6$ obtained on the assumption of a sixth-order method. With $h = \frac{1}{4}\pi$, a near-linear growth of the error norm is evident in the early stages but the behaviour of the global error becomes more erratic when the computed solution differs significantly from the true orbit.

A similar pattern was found in other cases. For the sixth-order Panovsky–Richardson method, for example, with $e = 0.1$, the error norm is again linear to better than graphical accuracy over 65 610 orbits with $h = \frac{1}{8}\pi$, and when $h = \frac{1}{4}\pi$ the increase is close to linear for 10 000 orbits. The fact that a graph of our results for $h = \frac{1}{4}\pi$ would be convincingly linear for 10 000 orbits suggests that caution is advisable in drawing conclusions about long-term behaviour, such as those of Okunbor [11], from numerical results for any arbitrarily chosen number of orbits.

Another feature of our results, which is evident from Table 5, is that at integral multiples of the orbital period, though not at all other times, the absolute error in the approximation for y $(= 1 - e)$ is very much less in magnitude than the error in the approximation for z $(= 0)$. However, whereas the global error in the z-approximation grows approximately linearly that in y-approximation grows more rapidly.

Our results show that over arbitrarily long time intervals the Panovsky–Richardson methods do not have the property of linear error growth for Kepler's problem, which the analysis of Calvo and Sanz-Serna [1] predicts for symplectic methods. However, the results indicate that, for sufficiently small steplengths, any nonlinearity in the error growth may take a very long time to become significant. We do not have an explanation for this distinction between these implicit, collocation-based Runge–Kutta–Nyström methods and some explicit RKN methods, such as the method of order 8 for which we gave results in Table 3 of [3].

8. Conclusion

We have shown that the two-step methods of Panovsky and Richardson [13], and those of a larger class which we call generalised Panovsky–Richardson methods, are equivalent to

collocation-based, one-step, Runge–Kutta–Nyström methods. The one-step version should be the preferred form in any implementation of these methods because of its advantages in starting the calculation, in any changes of steplength or order, and in its behaviour with respect to the propagation of rounding errors.

Acknowledgements

A.S. Booth was supported by a research studentship awarded by the Science and Engineering Research Council.

References

[1] M.P. Calvo and J.M. Sanz-Serna, The development of variable-step symplectic integrators, with applications to the two-body problem, *SIAM J. Sci. Comput.* **14** (1992) 936–952.
[2] J.P. Coleman, Rational approximation for the cosine function; P-acceptability and order, *Numer. Algorithms* **3** (1992) 143–158.
[3] J.P. Coleman and A.S. Booth, Analysis of a family of Chebyshev methods for $y'' = f(x, y)$, *J. Comput. Appl. Math.* **44** (1992) 95–114.
[4] C.R. de Boor and B. Swartz, Collocation at Gaussian points, *SIAM J. Numer. Anal.* **10** (1973) 582–606.
[5] L. Fox and I.B. Parker, *Chebyshev Polynomials in Numerical Analysis* (Oxford Univ. Press, Oxford, 1968).
[6] E. Hairer, S.P. Nørsett and G. Wanner, *Solving Ordinary Differential Equations I. Nonstiff Problems* (Springer, Berlin, 1987).
[7] P. Henrici, *Discrete Variable Methods in Ordinary Differential Equations* (Wiley, New York, 1962).
[8] J.P. Imhof, On the method for numerical integration of Clenshaw and Curtis, *Numer. Math.* **5** (1963) 138–141.
[9] L. Kramarz, Stability of collocation methods for the numerical solution of $y'' = f(x, y)$, *BIT* **20** (1980) 215–222.
[10] S.P. Nørsett, Collocation and perturbed collocation methods, in: G.A. Watson, Ed., *Numerical Analysis*, Lecture Notes in Math., Vol. 773 (Springer, Berlin, 1980).
[11] D. Okunbor, Variable step size does not harm second-order integrators for Hamiltonian systems, *J. Comput. Appl. Math.* **47** (1993) 273–275.
[12] D. Okunbor and R.D. Skeel, An explicit Runge–Kutta–Nyström method is canonical if and only if its adjoint is explicit, *SIAM J. Numer. Anal.* **29** (1992) 521–527.
[13] J. Panovsky and D.L. Richardson, A family of implicit Chebyshev methods for the numerical integration of second-order differential equations, *J. Comput. Appl. Math.* **23** (1988) 35–51.
[14] J.M. Sanz-Serna, Symplectic integrators for Hamiltonian problems: an overview, *Acta Numerica* (1992), 243–286.
[15] P.J. Van der Houwen, B.P. Sommeyer and Nguyen huu Chong, Stability of collocation-based Runge–Kutta–Nystrom methods, *BIT* **31** (1991) 469–481.